

Pentane

109-66-0 | DTXSID2025846

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 3.15

Global applicability domain: Inside

Local applicability domain index: 6.61e-01

Confidence level: 6.29e-01

Nearest Neighbors from the Training Set

Image not found

Pentane

Measured: 3.39

Predicted: 3.15

Image not found

n-Hexane

Measured: 3.90

Predicted: 3.96

Image not found

Butane

Measured: 2.89

Predicted: 2.79

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2-Methyl-2-butene

Measured: 2.67

Predicted: 2.67